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The Ground State of Bottomium to Two Loops and Higher*

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Abstract

We consider the properties of the ground state of bottomium. The Υ mass is evaluated to two loops, and including leading higher order $[O(\alpha_s^5 \log \alpha_s)]$ and m_c^2/m_b^2 corrections. This allows us to present updated values for the pole mass and $\overline{MS}$ mass of the b quark: $m_b = 5022 \pm 58$ MeV, for the pole mass, and $\bar{m}_b(\bar{m}_b) = 4286 \pm 36$ MeV for the $\overline{MS}$ one. The value for the $\overline{\mathrm{MS}}$ mass is accurate including and $O(\alpha_s^3)$ corrections and leading orders in the ratio m_c^2/m_b^2. We then consider the wave function for the ground state of $\bar{b}b$, which is calculated to two loops in the nonrelativistic approximation. Taking into account the evaluation of the matching coefficients by Beneke and Signer one can calculate, in principle, the width for the decay $\Upsilon \to e^+e^-$ to order α_s^5. Unfortunately, given the size of the corrections it is impossible to produce reliable numbers. The situation is slightly better for the ground state of toponium, where a decay width into e^+e^- of 11 – 14 keV is predicted.

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1. Introduction

In this paper we profit from the existence of recently obtained results on heavy quarkonium to give an accurate picture of the ground state of bottomium. In particular, we have the two loop relation between pole and $\overline{\mathrm{MS}}$ mass[1]; the $O(\alpha_s^5 \log \alpha_s)$ and $O(m_c^2/m_b^2)$ corrections to quarkonium potential[2]; and the two loop expression for the decay $\Upsilon \to e^+e^-$ in terms of the nonrelativistic ground state wave function[3], which last we evaluate here also to two loops.

All this allows us to give a determination of the pole mass of the b quark,

$$m_b = 5022 \pm 58 \ \mathrm{MeV}$$

correct up to and including α_s^4 and $O(\alpha_s^5 \log \alpha_s)$ corrections as well as leading nonperturbative and $O(m_c^2/m_b^2)$ ones; to find a value for the $\overline{\mathrm{MS}}$ mass,

$$\bar{m}_b(\bar{m}_b) = 4286 \pm 36 \ \mathrm{MeV}$$

correct to order α_s^3 and leading nonperturbative and $O(m_c^2/m_b^2)$; and to present an evaluation of the width

$$\Gamma(\Upsilon \to e^+e^-)$$

accurate to order α_s^5 and including leading nonperturbative contributions. The determination of the pole mass turns out to be very stable, in particular when comparing it with older determinations[4,5]. The $\overline{\mathrm{MS}}$ mass is less stable, but on the other hand is in good agreement with recent NNLO (next-to-next to leading order) evaluations based on QCD sum rules[6]. Finally, the values found for the width, while in rough agreement with experiment, show an excessive dependence both on the renormalization point chosen to calculate and on the degree of accuracy of the calculation: both due to the very large size of one and two loop corrections.

The plan of this paper is as follows. In Sect. 2 we present the hamiltonian used to obtain the results. This is used in Sect. 3 to evaluate pole mass and $\overline{\mathrm{MS}}$ mass for the b quark, and to comment on the convergence properties of the series. The decay rates to e^+e^- of the Υ are discussed in Sect. 4. The article is finished with an Appendix where some of the evaluations, which may be of interest for other problems, are presented in detail.

2. The nonrelativistic hamiltonian

In the static limit the $\bar{b}b$ interaction may be described by a potential. The ensuing hamiltonian may be written as

$$H = \widetilde{H}^{(0)} + H_1 \tag{2.1}$$

where

$$\widetilde{H}^{(0)} = 2m + \frac{-1}{m}\Delta - \frac{C_F \widetilde{\alpha}_s(\mu)}{r}; \tag{2.2a}$$

we have put together all coulomb-like pieces of the interaction so that

$$\widetilde{\alpha}_s(\mu^2) = \alpha_s(\mu^2)\left\{1 + c^{(1)}\frac{\alpha_s(\mu^2)}{\pi} + c^{(2)}\frac{\alpha_s^2}{\pi^2}\right\} \tag{2.2b}$$

$$\begin{aligned} c^{(1)} =& a_1 + \frac{\gamma_{\mathrm{E}}\beta_0}{2}, \\ c^{(2)} =& \gamma_{\mathrm{E}}\left(a_1\beta_0 + \frac{\beta_1}{8}\right) + \left(\frac{\pi^2}{12} + \gamma_{\mathrm{E}}^2\right)\frac{\beta_0^2}{4} + a_2 \end{aligned}$$

and[1,2]

$$\begin{aligned} a_1 =& \frac{31C_A - 20T_F n_f}{36}, \\ a_2 =& \tfrac{1}{16}\Big\{ \left[\tfrac{4343}{162} + 4\pi^2 - \tfrac{1}{4}\pi^4 + \tfrac{22}{3}\zeta_3\right] C_A^2 \\ & - \left[\tfrac{1798}{81} + \tfrac{56}{3}\zeta_3\right] C_A T_F n_f - \left[\tfrac{55}{3} - 16\zeta_3\right] C_F T_F n_f + \tfrac{400}{81} T_F^2 n_f^2 \Big\} \\ & \simeq 13.2. \end{aligned} \tag{2.2c}$$

The remaining piece of the interaction H_1 is, in the non-relativistic (static) limit,

$$H_1^{\rm NR} = V^{(L,1)} + V^{(L,2)} + V^{(LL)}, \tag{2.3a}$$

$$\begin{aligned} V^{(L,1)} =& \frac{-C_F\alpha_s(\mu^2)^2}{\pi}\,\frac{\beta_0}{2}\,\frac{\log r\mu}{r},\\ V^{(L,2)} =& \frac{-C_F\alpha_s^3}{\pi^2}\left(a_1\beta_0+\frac{\beta_1}{8}+\frac{\gamma_{\rm E}\beta_0^2}{2}\right)\frac{\log r\mu}{r},\\ V^{(LL)} =& \frac{-C_F\beta_0^2\alpha_s^3}{4\pi^2}\,\frac{\log^2 r\mu}{r}. \end{aligned} \tag{2.3b}$$

Note that the mass that appears in above formulas is the *pole* mass, but all other renormalization is carried in the $\overline{\rm MS}$ scheme. For more details on this see refs. 4, 5.

Eqs.(2.2) give what we will need to calculate the wave function, when taking into account also the results of Beneke et al.[3]; but for the spectrum we can do better. First, we have to add one loop velocity corrections. For the spin-independent part of the spectrum this is

$$H_{\text{vel. dep.}} = \frac{C_F b_1 \alpha_s^2}{2mr^2}, \tag{2.4a}$$

$b_1 = \frac{1}{2}(C_F - 2C_A)$ and a spin-dependent piece

$$V_{\rm hf} = \frac{4\pi C_F\alpha_s}{3m^2}s(s+1)\delta(\mathbf{r}) \tag{2.4b}$$

has to be added for vector states like the Υ. Then we have the corrections yielding contributions of order $\alpha_s^5\log\alpha_s$, which are the leading $O(\alpha_s^5)$ corrections in the limit of small α_s. They have been evaluated in ref. 2 and they lead to a correction on the mass of the υ of

$$\delta_{[\alpha_s^5\log\alpha_s]}E_{10} = -m[C_F+\tfrac{3}{2}C_A]C_F^4\alpha_s^5(\log\alpha_s)/\pi, \tag{2.5}$$

for $\mu = 2/a = mC_F\alpha_s$.

The influence of the nonzero mass of the c quark, the only worth considering, will be evaluated now. To leading order it only contributes to the $\bar{b}b$ potential through a c-quark loop in the gluon exchange diagram. The momentum space potential generated by a nonzero mass quark through this mechanism is then, in the nonrelativistic limit,

$$\widetilde{V}_{c\,\rm mass} = -\frac{8C_F T_F\alpha_s^2}{\mathbf{k}^2}\int_0^1 {\rm d}x\,x(1-x)\log\frac{m_c^2+x(1-x)\mathbf{k}^2}{\mu^2}. \tag{2.6}$$

We expand in powers of $m_c^2/\mathbf{k}^2$. The zeroth term is already included in (5). The first order correction is[2]

$$\delta_{c\,\rm mass}\widetilde{V} = -\frac{8C_F T_F\alpha_s^2 m_c^2}{\mathbf{k}^4}. \tag{2.7}$$

In x-space,

$$\delta_{c\,\rm mass}V = \frac{C_F T_F\alpha_s^2 m_c^2}{\pi}\,r. \tag{2.8}$$

If we are interested in a calculation correct to order α_s^4 and $\alpha_s^5\log\alpha_s$ for the bound state energies, or order α_s^5 for the decay rate, all these terms have to be treated as first order perturbations except $V^{(L,1)}$ that should be computed to second order.[1] Of course the hamiltonian $\widetilde{H}^{(0)}$ can, and will, be solved exactly.

3. The b quark mass

[1] In fact, this is the most difficult part of the calculation.

3.1. Pole mass

Here α_s is to be calculated to three loops:

$$\alpha_s(\mu) = \frac{4\pi}{\beta_0 L}\left\{1 - \frac{\beta_1 \log L}{\beta_0^2 L} + \frac{\beta_1^2 \log^2 L - \beta_1^2 \log L + \beta_2\beta_0 - \beta_1^2}{\beta_0^4 L^2}\right\} \tag{3.1}$$

with

$$L = \log\frac{\mu^2}{\Lambda^2};\quad \beta_0 = 11 - \tfrac{2}{3}n_f,\quad \beta_1 = 102 - \tfrac{38}{3}n_f,\quad \beta_2 = \tfrac{2857}{2} - \tfrac{5033}{18}n_f + \tfrac{325}{54}n_f^2.$$

We take as input parameters

$$\Lambda(n_f = 4,\ \text{three loops}) = 0.283 \pm 0.035\ \text{GeV}\ \left[\ \alpha_s(M_Z^2) \simeq 0.117 \pm 0.024\ \right]$$

(ref. 7) and for the gluon condensate, very poorly known, the value $\langle\alpha_s G^2\rangle = 0.06 \pm 0.02\ \text{GeV}^4$. From the mass of the Υ particle we have a very precise determination for the pole mass of the b quark. This determination is correct to order α_s^4 and including leading $O(m_c^2/m_b^2)$ and leading nonperturbative corrections as well as the α_s^5 corrections proportional to $\log\alpha_s$; the details of it will be given below. With the renormalization point $\mu = m_b C_F \alpha_s$ we have,

$$\begin{aligned} m_b =& 5022 \pm 43\,(\Lambda)\ \mp 5\,(\langle\alpha_s G^2\rangle)^{-31}_{+37}\ (\text{vary } \mu^2 \text{ by } 25\%)\ \pm 38\ (\text{other th. uncert.}) \\ =& 5022 \pm 58\ \text{MeV}\,. \end{aligned} \tag{3.2}$$

Here we append (Λ) to the error induced by that of Λ, and likewise $(\langle\alpha_s G^2\rangle)$ tags the error due to that of the condensate. The error labeled (other th. uncert.) includes also the error evaluated in ref. 8; the rest is as in ref. 5.

We collect in the table the determinations of the b quark mass based on spectroscopy, to increasing accuracy. The *stability* of the numerical values of the pole mass is remarkable: the pole masses all lie within each other error bars. The $\overline{\text{MS}}$ ones (that will be discussed in greater detail in next subsection) show more spread. It may be noted that the three loop value for $\bar{m}_b(\bar{m}_b^2)$, 4286 ± 36, agrees perfectly with the Beneke–Signer three loop result[6] based on sum rules, $\bar{m}_b(\bar{m}_b^2) = 4260 \pm 100$ MeV. This agreement, however, is less satisfactory than it would appear at first sight because of the large size of the $O(\alpha_s^3)$ corrections. We will discuss this more in next subsection.

Reference	m_b(pole)	$\bar{m}_b(\bar{m}_b^2)$	m_c(pole)	$\bar{m}_c(\bar{m}_c^2)$
TY	4971 ± 72	4401^{+21}_{-35}	1585 ± 20 (*)	1321 ± 30 (*)
PY	5065 ± 60	4455^{+45}_{-29}	1866^{+215}_{-133}	1542^{+163}_{-104}
Here	5022 ± 58	4286 ± 36	–	–

TABLE 1. b and c quark masses. (*) Systematic errors not included.

TY: Titard and Ynduráin[4]. $O(\alpha_s^3)$ plus $O(\alpha_s^3)v$, $O(v^2)$ for m; $O(\alpha_s^2)$ for $\bar{m}$. Rescaled for $\Lambda(n_f = 4) = 283$ MeV.
PY: Pineda and Ynduráin[5]. Full $O(\alpha_s^4)$ for m; $O(\alpha_s^2)$ for $\bar{m}$. Rescaled for $\Lambda(n_f = 4) = 283$ MeV.
Here: This calculation. $O(\alpha_s^4)$, $O(\alpha_s m_c^2/m_b^2)$ and $O(\alpha_s^5\log\alpha_s)$ for m; $O(\alpha_s^3)$ and $O(\alpha_s^2 m_c^2/m_b^2)$ for $\bar{m}$. Values not given for the c quark, as the higher order terms are as large as the leading ones.

We finally remark that the values of m_b quoted e.g. in the Table 1 were *not* obtained solving Eq. (8), but solving exactly the coulombic part of the interaction, and perturbing the result (see refs. 4, 5 for details). We also note that, in the determinations of m_b, the new pieces, $O(\alpha_s m_c^2/m_b^2)$ and $O(\alpha_s^5\log\alpha_s)$, have been evaluated to first order; in particular, we have included the corresponding shifts in the *central* values, not in the errors. If we included these, the errors would decrease by some 7%.

3.2. $m_b - \bar{m}_b(\bar{m}_b)$ connection

The connection of the pole mass with the $\overline{\text{MS}}$ mass has been known for some time to one and two loops: very recently, a three loop evaluation has been completed. Coupling this with the pole mass evaluations, we now have an order α_s^3 result for the $\overline{\text{MS}}$ mass. We review here briefly this.

Write, for a heavy quark,

$$\bar{m}(\bar{m}) \equiv m/\{1+\delta_1+\delta_2+\delta_3+\cdots\}; \tag{3.3a}$$

m here denotes the *pole* mass, and $\bar{m}$ is the $\overline{\rm MS}$ one. One has

$$\delta_1 = C_F\frac{\alpha_s(\bar{m})}{\pi}, \quad \delta_2 = c_2\left(\frac{\alpha_s(\bar{m})}{\pi}\right)^2, \quad \delta_3 = c_3\left(\frac{\alpha_s(\bar{m})}{\pi}\right)^3. \tag{3.3b}$$

The coefficient c_2 has been evaluated by Gray et al.[1], and reads

$$c_2 = -K + 2C_F, \tag{3.3c}$$

$$\begin{aligned} K = K_0 + \sum_{i=1}^{n_f} \Delta\left(\frac{m_i}{m}\right), \quad & K_0 = \tfrac{1}{9}\pi^2\log 2 + \tfrac{7}{18}\pi^2 - \tfrac{1}{6}\zeta(3) + \tfrac{3673}{288} - \left(\tfrac{1}{18}\pi^2 + \tfrac{71}{144}\right)(n_f+1) \\ \simeq 16.11 - 1.04\, n_f; \quad & \Delta(\rho) = \tfrac{4}{3}\left[\tfrac{1}{8}\pi^2\rho - \tfrac{3}{4}\rho^2 + \cdots\right]. \end{aligned} \tag{3.3d}$$

m_i are the (pole) masses of the quarks strictly lighter than m, and n_f is the number of these. For the b quark case, $n_f = 4$ and only the c quark mass has to be considered; we will take $m_c = 1.8$ GeV (see Table 1 above) for the calculations.

The coefficient c_3 was recently calculated by Melnikov and van Ritbergen[1]. Neglecting now the m_i,

$$c_3 \simeq 190.389 - 26.6551 n_f + 0.652694 n_f^2. \tag{3.3e}$$

For the b, c quarks, with α_s as given before,

$$\begin{aligned} \delta_1(b) =& 0.090, \quad \delta_1(c) = 0.137, \\ \delta_2(b) =& 0.045, \quad \delta_2(c) = 0.108, \\ \delta_3(b) =& 0.029; \quad \delta_3(c) = 0.125. \end{aligned} \tag{3.4}$$

From these values we conclude that, for the c quark, the series has started to diverge at second order, and it certainly diverges at order α_s^3. For the b quark the series is at the edge of convergence for the α_s^3 contribution.

Using the three loop relation (3.3) of the pole mass to the $\overline{\rm MS}$ mass we then find, from the results in Subsect. 3.1 for the pole mass, the value

$$\bar{m}_b(\bar{m}_b) = 4284 \pm 7\ (\Lambda) \mp 5\ (\langle\alpha_s G^2\rangle) \pm 35\ (\text{other th. uncert.}) = 4284 \pm 36\ \text{MeV}. \tag{3.5}$$

This is the value incorporated in Table 1. The slight dependence of $\bar{m}$ on Λ when evaluated in this way was already noted in ref. 4.

There is another way of obtaining $\bar{m}$, which is to express directly the mass of the Υ in terms of it, using Eq. (3.3) and the order α_s^3 formula for the Υ mass in terms of the pole mass Eq. (3.3a). One finds, for $n_f = 4$, and neglecting m_c^2/m_b^2,

$$\begin{aligned} M(\Upsilon) =& 2\bar{m}(\bar{m})\Bigg\{1 + C_F\frac{\alpha_s(\bar{m})}{\pi} + 7.559\left(\frac{\alpha_s(\bar{m})}{\pi}\right)^2 \\ &+ \Big[66.769 + 18.277\left(\log C_F + \log\alpha_s(\bar{m})\right)\Big]\left(\frac{\alpha_s(\bar{m})}{\pi}\right)^3\Bigg\}. \end{aligned} \tag{3.6a}$$

(One could add the leading nonperturbative contributions to (3.6a) à la Leutwyler–Voloshin in the standard way). This method has been at times advertised as improving the convergence, allegedly because the $\overline{\rm MS}$ mass does not suffer from nearby renormalon singularities. But a close look to (3.6a) does not seem to bear this out. To an acceptable $O(\alpha_s^4)$ error we can replace $\log(\alpha_s(\bar{m}))$ by $\log(\alpha_s(M(\Upsilon/2))$ above. With Λ as before (3.6a) then becomes

$$M(\Upsilon) = 2\bar{m}_b(\bar{m}_b)\left\{1 + C_F\frac{\alpha_s(\bar{m})}{\pi} + 7.559\left(\frac{\alpha_s(\bar{m})}{\pi}\right)^2 + 43.502\left(\frac{\alpha_s}{\pi}\right)^3\right\}. \tag{3.6b}$$

This does not look particularly convergent, and is certainly not an improvement over the expression using the pole mass where one has, for the choice $\mu = C_F m_b \alpha_s$ and still neglecting the masses of quarks lighter than the b,

$$M(\Upsilon) = 2m_b \left\{1 - 2.193\left(\frac{\alpha_s(\mu)}{\pi}\right)^2 - 24.725\left(\frac{\alpha_s(\mu)}{\pi}\right)^3 - 458.28\left(\frac{\alpha_s(\mu)}{\pi}\right)^4 + 897.93\,[\log\alpha_s]\left(\frac{\alpha_s}{\pi}\right)^5\right\}. \tag{3.7}$$

To order three, (3.7) is actually better[2] than (3.6b). What is more, logarithmic terms appear in (3.6) at order α_s^3, while for the pole mass expression they first show up at order α_s^5. Finally, the direct formula for $M(\Upsilon)$ in terms of the $\overline{\mathrm{MS}}$ mass presents the extra difficulty that the *nonperturbative* contribution becomes larger than than what one has for the expression in terms of the pole mass (~ 80 against ~ 9 MeV), because of the definition of the renormalization point. With the purely perturbative expression (3.6) plus leading nonperturbative (gluon condensate) correction one finds the value $\bar{m}_b(\bar{m}_b) = 4167\,\mathrm{MeV}$, rather low.

4. The Decay Rates $\Upsilon \to e^+e^-$ and $T \to e^+e^-$

For bound state calculations it is convenient to solve $\widetilde{H}^{(0)}$ exactly, and treat H_1 as a perturbation; but, to evaluate the wave function it is preferable to work in the following somewhat different manner. Define the quantities

$$a \equiv \frac{2}{mC_F\alpha_s(\mu)}, \quad \rho \equiv \frac{2r}{a}.$$

One may rewrite H_1 as

$$\begin{aligned}
H_1 &= H_{1C} + H_{1L}^{(1)} + H_{1L}^{(2)} + H_{1LL};\\
H_{1C} &= \left(\log\frac{\mu a}{2}\right)\left\{\tfrac{1}{2}\beta_0\frac{\alpha_s(\mu)}{\pi} + \left[c_L + \frac{\beta_0^2\log\mu a/2}{4}\right]\frac{\alpha_s^2(\mu)}{\pi^2}\right\}\frac{-C_F\alpha_s(\mu)}{r}\\
H_{1L}^{(1)} &= -\frac{2}{a}\,\frac{C_F\beta_0\alpha_s^2(\mu)}{2\pi}\,\frac{\log\rho}{\rho};\\
H_{1L}^{(2)} &= -\frac{2}{a}\left[c_L + \frac{\beta_0^2}{2}\log\frac{\mu a}{2}\right]\frac{C_F\alpha_s^3(\mu)}{\pi^2}\,\frac{\log\rho}{\rho};\\
H_{1LL} &= -\frac{2}{a}\,\frac{C_F\beta_0^2\alpha_s^3}{4\pi^2}\,\frac{\log\rho}{\rho}.
\end{aligned} \tag{4.1}$$

Here $c_L = a_1\beta_0 + \frac{1}{8}\beta_1 + \gamma_E\beta_0^2/2$.

One can put $\widetilde{H}^{(0)}$ and H_{1C} together, $\bar{H}^{(0)} = \widetilde{H}^{(0)} + H_{1C}$, and solve the corresponding coulombic Schrödinger equation exactly by just replacing, in the ordinary solution of the coulombic problem,

$$\begin{aligned}
H^{(0)}\Psi_{nl}^{(0)}(\mathbf{r}) &= E_n^{(0)}\Psi_{nl}^{(0)}(\mathbf{r}),\\
H^{(0)} &= -\frac{1}{m}\Delta - \frac{C_F\alpha_s}{r},\\
\Psi_{nl}^{(0)}(\mathbf{r}) &= \frac{1}{\sqrt{4\pi}}R_{nl}^{(0)}(r), \quad R_{10}^{(0)}(r) = \alpha_s^{3/2}\frac{(mC_F)^{3/2}}{\sqrt{2}}\mathrm{e}^{-rC_F m\alpha_s/2},
\end{aligned} \tag{4.2}$$

the coupling α_s according to

$$\alpha_s \to \alpha_s\left\{1 + c^{(1)}\frac{\alpha_s(\mu^2)}{\pi} + c^{(2)}\frac{\alpha_s^2}{\pi^2} + \left(\log\frac{\mu a}{2}\right)\left[\tfrac{1}{2}\beta_0\frac{\alpha_s(\mu)}{\pi} + \left(c_L + \frac{\beta_0^2\log\mu a/2}{4}\right)\frac{\alpha_s^2(\mu)}{\pi^2}\right]\right\}.$$

The remaining $H_{1L}^{(2)} + H_{1LL}$ can then be evaluated as first order perturbations; only $H_{1L}^{(1)}$ has to be calculated to first and second order and, for this second order, the fact that one perturbs on $\bar{H}^{(0)}$ has also to be taken into account.

[2] The convergence of Eq. (3.7) is still improved if one solves exactly the purely coulombic part of the static potential, as was done in Subsect. 3.1. For example, the $O(\alpha_s^4)$ term would become $-232.12(\alpha_s/\pi)^4$.

4.1 Calculation of perturbations

The NNLO (two loop) hard part of the radiative correction to the leptonic decay of quarkonium, say

$$\Gamma(\Upsilon \to e^+e^-),$$

has been evaluated some time ago[3]. One can then write

$$\Gamma(\Upsilon \to e^+e^-) = \left[\frac{Q_b \alpha_{\rm QED}}{M(\Upsilon)}\right] \left|\left\{1 + \delta^{(1)}_{\rm hard}\frac{\alpha_s(\mu)}{\pi} + \delta^{(2)}_{\rm hard}\frac{\alpha_s^2(\mu)}{\pi^2}\right\} R_{10}(0)\right|^2, \tag{4.3a}$$

where[1]

$$\begin{aligned}
\delta^{(1)}_{\rm hard} =& -2C_F,\\
\delta^{(2)}_{\rm hard} =& C_F^2\left\{\pi^2\left[\tfrac{1}{6}\log\frac{m^2}{\mu^2} - \tfrac{79}{36} + \log 2\right] + \tfrac{23}{8} - \tfrac{1}{2}\zeta_3\right\}\\
&+C_F C_A\left\{\pi^2\left[\tfrac{1}{4}\log\frac{m^2}{\mu^2} + \tfrac{89}{144} - \tfrac{5}{6}\log 2\right] - \tfrac{151}{72} - \tfrac{13}{4}\zeta_3\right\}\\
&+\tfrac{11}{18}C_F T_F n_f + C_F T_F\left(-\tfrac{2}{9}\pi^2 + \tfrac{22}{9}\right)\\
&+\frac{C_F \beta_0 \log m^2/\mu^2}{2},
\end{aligned} \tag{4.3b}$$

and $R_{10}(0)$ is the static (radial) wave function, i.e., evaluated neglecting terms of relative order $1/m$ in the interaction. We will write

$$R_{10}(0) = \left\{1 + \delta^{(1)}_{\rm wf}\frac{\alpha_s(\mu)}{\pi} + \delta^{(2)}_{\rm wf}\frac{\alpha_s^2(\mu)}{\pi^2} + \delta_{\rm NP}\right\} R^{(0)}_{10}(0); \tag{4.3c}$$

$R^{(0)}_{10}(0)$ is as in (4.2) and the $\delta_{\rm wf}$ are to be evaluated with H in (2.1) (or (4.1)). Finally, the (leading) nonperturbative piece $\delta_{\rm NP}$ may be obtained in terms of the gluon condensate $\langle\alpha_s G^2\rangle$ as in refs. 4, 9 so that

$$\delta_{\rm NP} = \frac{2\,968\pi\langle\alpha_s G^2\rangle}{425 m^4 (C_F\widetilde{\alpha}_s)^6}. \tag{4.4}$$

Define then, with self-explanatory notation,

$$\delta^{(1)}_{\rm wf}\frac{\alpha_s}{\pi} + \delta^{(2)}_{\rm wf}\left(\frac{\alpha_s}{\pi}\right)^2 = \Delta_C + \Delta^{(1)}_{L,1} + \Delta^{(1)}_{L,2} + \Delta^{(1)}_{LL} + \Delta^{(2)}_{L,1}. \tag{4.5}$$

Δ_C is calculated trivially, as it is equivalent to a modification of the coulombic potential in $H^{(0)}$. The remaining δs are easily evaluated with the formulas of the Appendix. We find,

$$\begin{aligned}
\Delta_C =& \tfrac{3}{2}\left[c_1 + \frac{\beta_0\log\mu a/2}{2}\right]\frac{\alpha_s(\mu)}{\pi}\\
&+\left\{\tfrac{3}{8}\left[c_1 + \frac{\beta_0\log\mu a/2}{2}\right]^2 + \tfrac{3}{2}\left[c_2 + 2c_L\log\frac{a\mu}{2} + \frac{\beta_0^2\log^2 a\mu/2}{4}\right]\frac{\alpha_s^2}{\pi^2}\right\};
\end{aligned} \tag{4.6a}$$

$$\begin{aligned}
\Delta^{(1)}_{L,1} =& -\frac{3\beta_0\alpha_s(\mu)}{4\pi}\left(\gamma_{\rm E} + \frac{\pi^2-6}{9}\right) + 3\beta_0\left(\gamma_{\rm E} + \frac{\pi^2-6}{9}\right)\left(c^{(1)} + \frac{\beta_0\log a\mu/2}{2}\right)\frac{\alpha_s^2(\mu)}{4\pi^2};\\
\Delta^{(1)}_{L,2} =& -3\left(\gamma_{\rm E} + \frac{\pi^2-6}{9}\right)\left[2c_L + \beta_0^2\log\frac{a\mu}{2}\right]\frac{\alpha_s^2(\mu)}{4\pi^2};\\
\Delta^{(1)}_{LL} =& \beta_0^2\left\{2\zeta_3 - (1-\gamma_{\rm E})\left(1 + \frac{\pi^2}{3}\right) + \tfrac{3}{2}\left[\gamma_{\rm E}^2 - 2\gamma_{\rm E} + \frac{\pi^2}{6}\right]\right\}\frac{\alpha_s^2(\mu)}{4\pi},
\end{aligned} \tag{4.6b}$$

where $\Delta^{1)}_{L,1}$ above actually contains the NNLO mixed coulombic-logarithmic correction. Finally,

$$\Delta^{(2)}_{L,1} = c^{(2)}_{L,1}\frac{\beta_0^2\alpha_s^2}{4\pi^2}, \qquad c^{(2)}_{L,1} \simeq 1.75. \tag{4.6c}$$

For the exact value of $c^{(2)}_{L,1}$, see the Appendix, Eqs. (A9). This finishes the calculation of the decay rate.

4.2 NLO calculation

Using (4.1-6) to one loop only we find the NLO result,

$$\Gamma(\Upsilon \to e^+e^-) = \left\{1 + \left[\frac{3\beta_0}{4}\left(\log\frac{a\mu}{2} - \gamma_{\rm E} + \frac{6-\pi^2}{9}\right) + \tfrac{3}{2}\left(\frac{\gamma_{\rm E}\beta_0}{2} + \frac{93-10n_f}{36}\right) - 2C_F\right]\frac{\alpha_s}{\pi}\right\} \times\Gamma^{(0)}(\Upsilon \to e^+e^-) \tag{4.7}$$

where the LO expression $\Gamma^{(0)}$ is

$$\Gamma^{(0)} = 2\left[\frac{Q_b\alpha_{\rm QED}}{M(\Upsilon)}\right][mC_F\alpha_s(\mu)]^3.$$

We note that (4.7) is slightly different from the result obtained using a variational method (instead of Rayleigh–Schrödinger perturbation theory) to evaluate δR_{10}, which gives

$$\Gamma(\Upsilon \to e^+e^-) = \left\{1 + \left[\frac{3\beta_0}{4}\left(\log\frac{a\mu}{2} - \gamma_{\rm E}\right) + \tfrac{3}{2}\left(\frac{\gamma_{\rm E}\beta_0}{2} + \frac{93-10n_f}{36}\right) - 2C_F\right]\frac{\alpha_s}{\pi}\right\}\Gamma^{(0)}(\Upsilon \to e^+e^-).$$

4.3 NNLO calculation, and numerical results

The NNLO result is obtained with the full (4.3) – (4.6) expressions, with which numerical results are readily obtained. We select the values of the basic parameters $\Lambda(n_f = 4$, three loops), $\langle\alpha_s G^2\rangle$ as before. For the renormalization point there are two "natural" choices:

$$\mu_1 = m_b \quad \text{and} \quad \mu_2 = 2/a = 2.866\ \text{GeV}\,.$$

The first value gives a reasonable value for the width, These are the input values taken for the calculations reported in the Table 2 below.

$\Gamma(\Upsilon \to e^+e^-)$	LO	NLO	NNLO
$\mu = m$	0.41	1.22	1.13 keV
$\mu = 2/a$	0.73	0.55	0.80 keV

TABLE 2: Determination of $\Gamma(\Upsilon \to e^+e^-)$ to increasing accuracy.

The experimental figure is

$$\Gamma(\Upsilon \to e^+e^-) = 1.32 \pm 0.04\ \text{keV}\,.$$

Clearly, the large NLO and NNLO perturbative corrections, both of similar size, and of the leading NP correction, make the theoretical result unstable, as the Table shows.

For the (perhaps measurable) toponium (T) width we get, for $m_t = 175$ GeV, the corresponding results, summarized in Table 3.

$\Gamma(T \to e^+e^-)$	LO	NLO	NNLO
$\mu = m_t$	6.86	10.53	13.0
$\mu = 2/a$	10.24	10.91	13.5

TABLE 3: Determination of $\Gamma(T \to e^+e^-)$ to increasing accuracy.

The situation has improved with respect to what we had for bottomium, but the dependence on the renormalization point and on the order of perturbation theory considered is still a bit large. We can however conclude on an *estimate* of some 11.0 − 14 keV for the width.

Appendix: Perturbation by terms $\rho^{-1}\log^n\rho$

To obtain the result of perturbations by terms $\rho^{-1}\log^n\rho$ we first evaluate the perturbation by a term ρ^ν, ν = integer, continue to noninteger ν and differentiate with respect to ν at $\nu=-1$. For this we use the method devised by Leutwyler[5] and extended in the second paper of ref 5, Appendix, in general. The basic formula is the inversion formula

$$\frac{1}{E_1^{(0)}-H^{(0)}(\kappa)}\rho^\mu R_{10}(\rho)=\frac{ma^2}{4}\frac{\Gamma(\mu+2)\Gamma(\mu+3)}{\Gamma(\mu+3-\kappa)}\left(\sum_{j=0}^{\mu+1}\frac{\Gamma(j+1-\kappa)}{\Gamma(j+1)\Gamma(j+2)}\rho^j\right)R_{10}(\rho);$$

here

$$H(\kappa)=H_0+\frac{\kappa C_F\alpha_s}{r},\qquad R_{10}(\rho)=\frac{2}{a^{3/2}}\mathrm{e}^{-\rho/a}$$

with H_0 the free hamiltonian and $a=2/mC_F\alpha_s$. This inversion formula is valid for any κ and integer μ. Using this one may then check that the first order perturbation by ρ^ν, $\delta_{(\nu)}R_{10}$, is

$$\begin{aligned}\delta_{(\nu)}R_{10}(\rho)=P_{10}\frac{1}{E_1^{(0)}-H^{(0)}}P_{10}\rho^\nu R_{10}=-\frac{ma^2}{4}\Gamma(\nu+3)\\ \times\left\{\tfrac{3}{2}-\tfrac{1}{2}\rho-\left[\frac{\nu+1}{2}+\psi(\nu+2)-\psi(1)\right]+\sum_{j=1}^{\nu+1}\frac{\rho^j}{j\Gamma(j+2)}\right\}R_{10}(\rho).\end{aligned}\tag{A1}$$

Sums like that in (A1) may be continued to arbitrary ν by using the formula

$$\sum_{j=1}^{\nu+1}f(j)=\sum_{j=1}^{\infty}\left[f(j)-f(j+\nu+1)\right].\tag{A2}$$

This replacement is valid provided the sum $\sum_{j=1}^\infty f(j)$ is convergent; otherwise, we have to separate from f the leading, next to leading... pieces, to be summed explicitely, leaving a residue for which the sum up to infinity converges. This has already been done in getting (A1). As a check of this, we mention that the result agrees, for $\nu=-1$, with the result of the (trivial) evaluation obtained directly by replacing the coulombic potential according to

$$\frac{\kappa C_F\alpha_s}{r}\to\frac{\kappa C_F\alpha_s}{r}+\frac{1}{\rho}$$

and expanding: $\delta_{(-1)}R_{10}(\rho)=-(ma^2/4)(\frac{3}{2}-\frac{1}{2}\rho)R_{10}(\rho)$. The results of first order perturbation by $\rho^{-1}\log\rho$, $\rho^{-1}\log^2\rho$ are then found by differentiating (A1) with respect to ν.

To second order we require

$$\bar{\delta}^2_{(\lambda\nu)}R_{10}=\delta^2_{1(\lambda\nu)}R_{10}-\delta^2_{2(\lambda\nu)}R_{10},$$

$$\delta^2_{1(\lambda\nu)}R_{10}=P_{10}\frac{1}{E_1^{(0)}-H^{(0)}}P_{10}\rho^\lambda P_{10}\frac{1}{E_1^{(0)}-H^{(0)}}P_{10}\rho^\nu R_{10}$$

and

$$\delta^2_{2(\lambda\nu)}R_{10}=\langle R_{10}|\rho^\mu|R_{10}\rangle\,P_{10}\frac{1}{E_1^{(0)}-H^{(0)}}P_{10}\frac{1}{E_1^{(0)}-H^{(0)}}P_{10}\rho^\nu R_{10}.$$

Here P_{10} is the projector $P_{10}=1-|R_{10}\rangle\langle R_{10}|$. At $\rho=0$ we then have,

$$\begin{aligned}\delta^2_{1(\lambda\nu)}R_{10}(0)=&-\tfrac{1}{2}\left(\frac{ma^2}{4}\right)^2\Gamma(\nu+3)\\&\times\Bigg\{3\Bigg[-\Gamma(\lambda+3)\left[\tfrac{3}{2}-\left(\frac{\nu+1}{2}+\psi(\nu+2)-\psi(1)\right)\right]+\frac{\Gamma(4+\lambda)}{2}-\Phi(\lambda,\nu)\Bigg]\\&+2\Gamma(3+\lambda)\left[\tfrac{3}{2}-\left(\frac{\nu+1}{2}+\psi(\nu+2)-\psi(1)\right)\right]\left(\frac{\lambda+1}{2}+\psi(\lambda+2)-\psi(1)\right)\\&-\tfrac{1}{2}\frac{\Gamma(\lambda+5)}{\lambda+2}-\Gamma(\lambda+4)\left[\frac{\lambda+1}{2}+\psi(\lambda+2)-\psi(1)\right]+\Psi(\lambda,\nu)\Bigg\}R_{10}(0),\end{aligned}\tag{A3a}$$

and the functions Ψ, Φ are defined as

$$\begin{aligned}\Phi(\lambda,\nu)=&\sum_{j=1}^{\nu+1}\frac{\Gamma(j+\lambda+3)}{j\Gamma(j+2)}\\\Psi(\lambda,\nu)=&\sum_{j=1}^{\nu+1}\frac{\Gamma(j+\lambda+3)}{j\Gamma(j+2)}\left[j+\lambda+1+2\left(\psi(j+\lambda+2)-\psi(1)\right)\right]\\=&\sum_{j=1}^{\nu+1}\frac{\Gamma(j+\lambda+3)}{j\Gamma(j+2)}\left[\lambda+1+2\left(\psi(j+\lambda+2)-\psi(1)\right)\right]\\&+\frac{\Gamma(\lambda+\nu+5)}{(\lambda+2)\Gamma(\nu+3)}-\Gamma(\lambda+2)-\Gamma(\lambda+3),\end{aligned}\tag{A3b}$$

for ν, $\lambda=$ integer. The second expression for Ψ is obtained by using the identity[10]

$$\sum_{k=0}^{\mu}\binom{n+k}{k}=\binom{n+\mu+1}{n+1},\tag{A4}$$

and has the advantage that it can be continued directly with the use of (A2).

We will require the following results:

$$\begin{aligned}\frac{\partial^2}{\partial\nu\partial\lambda}\Phi(\lambda,\nu)\Big|_{\lambda=\nu=-1}=&\sum_{j=1}^{\infty}\frac{\psi(j+2)-j\psi'(j+2)}{j^2}\\=&\,\zeta_3+1-\frac{\pi^2\gamma_{\rm E}}{6};\\\frac{\partial^2}{\partial\nu\partial\lambda}\Psi(\lambda,\nu)\Big|_{\lambda=\nu=-1}=&\frac{\pi^2}{2}-2-\gamma_{\rm E}\\-\sum_{j=1}^{\infty}\Big\{2j\left[\psi''(j+1)+\psi'(j+1)\psi(j+2)\right]&+2\left(j\psi'(j+2)-\psi(j+2)\right)\left[\psi(j+1)-\psi(1)\right]\\&-2\psi'(j+1)-1\Big\}/j^2.\end{aligned}\tag{A5}$$

With the same methods we find,

$$\delta^2_{2(\lambda\nu)}R_{10}=-\tfrac{1}{4}\Gamma(\nu+3)\Gamma(\lambda+3)\left(\frac{ma^2}{4}\right)^2\left\{6\left[\tfrac{3}{2}-\left(\frac{\nu+1}{2}+\psi(\nu+2)-\psi(1)\right)\right]-15+\Psi(0,\nu)\right\}R_{10}(0),\tag{A6}$$

and we will need $\partial\Psi(0,\nu)/\partial\nu|_{\nu=-1}$. Write

$$\Psi(0,\nu)=-3+\frac{(\nu+4)(\nu+3)}{2}+\nu+1+2\left[\psi(\nu+2)-\psi(1)\right]+2\sum_{j=1}^{\nu+1}\left[\psi(j+2)-\psi(1)\right]+4\sum_{j=1}^{\nu+1}\frac{\psi(j+2)-\psi(1)}{j}.\tag{A7a}$$

With (cf. ref. 11 for some of the harmonic-type sums here[3])

$$\begin{aligned}\frac{\partial}{\partial\nu}\sum_{j=1}^{\nu+1}[\psi(j+2)-\psi(1)]\Big|_{\nu=-1}=&\frac{\pi^2}{3}-2,\\ \frac{\partial}{\partial\nu}\sum_{j=1}^{\nu+1}\frac{\psi(j+2)-\psi(1)}{j}\Big|_{\nu=-1}=&\zeta_3+1\end{aligned}\tag{A7b}$$

we find

$$\frac{\partial\Psi(0,\nu)}{\partial\nu}=4\,(\zeta_3+1)+\pi^2-1/2.\tag{A7c}$$

The function

$$\bar{R}_{10}=R_{10}+\delta_{(\nu)}R_{10}+\bar{\delta}^2_{(\lambda\nu)}R_{10}$$

is not normalized to unity. The normalized wave function is $\hat{R}_{10}=\|\bar{R}_{10}\|^{-1/2}\bar{R}_{10}$. Because R_{10} is orthogonal to $\delta_\nu R_{10}$, $\bar{\delta}^2_{\lambda\nu}R_{10}$ the normalization factor is

$$\|\bar{R}_{10}\|^{-1}=\left\{1+(\delta_{(\nu)}R_{10}|\delta_{(\lambda)}R_{10})\right\}^{-1/2}\simeq 1-\tfrac{1}{2}(\delta_{(\nu)}R_{10}|\delta_{(\lambda)}R_{10}).$$

Therefore, we have to correct $\bar{\delta}^2_{(\lambda\nu)}R_{10}$ for this and define

$$\begin{aligned}\delta^2_{(\lambda\nu)}R_{10}=&\bar{\delta}^2_{(\lambda\nu)}R_{10}+\delta^2_{\mathrm{norm.}(\lambda\nu)}R_{10},\\ \delta^2_{\mathrm{norm.}(\lambda\nu)}R_{10}=&-\tfrac{1}{2}(\delta_{(\nu)}R_{10}|\delta_{(\lambda)}R_{10})=-\frac{\Gamma(\lambda+3)\Gamma(\nu+3)}{2}\left(\frac{ma^2}{4}\right)^2\\ &\times\Bigg\{\tfrac{3}{4}+\tfrac{3}{2}\left[\frac{\lambda+1}{2}+\psi(\lambda+2)-\psi(1)+\frac{\nu+1}{2}+\psi(\nu+2)-\psi(1)\right]\\ &-\left[\frac{\lambda+1}{2}+\psi(\lambda+2)-\psi(1)\right]\left[\frac{\nu+1}{2}+\psi(\nu+2)-\psi(1)\right]\\ &-\tfrac{1}{4}\Big[\frac{(\nu+1)(\nu+2)+(\lambda+1)(\lambda+2)}{2}+5(\nu+\lambda-2)\\ &+6\Big(\psi(\nu+2)+\psi(\lambda+2)-2\psi(1)\Big)\Big]+\tfrac{1}{2}\sum_{j=1}^{\nu+1}\sum_{k=1}^{\lambda+1}\frac{\Gamma(j+k+3)}{j\Gamma(j+2)k\Gamma(k+2)}\Bigg\}R_{10}.\end{aligned}\tag{A8}$$

The only difficult point is the continuation of the double sum

$$S_{\lambda\nu}=\sum_{j=1}^{\nu+1}\sum_{k=1}^{\lambda+1}\frac{\Gamma(j+k+3)}{j\Gamma(j+2)k\Gamma(k+2)}$$

which diverges if using directly (A2). We avoid this by resorting again to the identity (A4). With it, we get $S_{\lambda\nu}=S^{(1)}_{\lambda\nu}+S^{(1)}_{\nu\lambda}$,

$$\begin{aligned}S^{(1)}_{\lambda\nu}=&\psi(\nu+3)+\psi(\lambda+3)-2\psi(\lambda+2)-2-2\Big[\sum_{k=2}^{\lambda+1}\frac{1}{k(k^2-1)}+\sum_{k=2}^{\lambda+1}\frac{1}{k^2}+1\Big]+(\nu+3)\left(2+\frac{\nu}{4}\right)\\ &+\frac{1}{\Gamma(\nu+3)}\sum_{k=2}^{\lambda+1}\left[\frac{2\Gamma(\nu+k+2)}{k-1}+\frac{2\Gamma(\nu+k+3)}{k}+\frac{2\Gamma(\nu+k+4)}{k+1}\right]\frac{1}{k\Gamma(k+2)},\end{aligned}$$

which can now be continued with (A2).

[3] The sum $\sum_{j=1}^{\nu+1}[\psi(j+2)-\psi(1)]$ can be evaluated exactly using the identity (A4) differentiated with respect to n at $n=0$. The derivative with respect to ν of the sum $\sum_{j=1}^{\nu+1}\dfrac{\psi(j+2)-\psi(1)}{j}$, being only logarithmically divergent, can be calculated with (A2).

For our calculation, we need to evaluate

$$\frac{\partial^2}{\partial\nu\partial\lambda} S_{\lambda\nu}\Big|_{\nu=\lambda=-1}.$$

The only nontrivial piece is the apparently divergent one arising for $k=2$. To get it, we note that

$$\frac{\partial^2}{\partial\nu\partial\lambda}\frac{1}{\Gamma(\nu+3)}\frac{2\Gamma(\nu+\lambda+k+2)}{(\lambda+k)(\lambda+k-1)\Gamma(\lambda+k+2}\Big|_{k=2,\nu=\lambda=-1} = \tfrac{3}{2}\psi'(2)-\tfrac{1}{2}\psi''(2)=\pi^2/2+2\zeta_3-5.$$

It is possible also to check some of the calculations here in two respects. First, we may evaluate the second order correstion to the energy shift by H_{1L}. This is given by

$$\delta_{1L}^{(2)}E_{10}=\left(\frac{2}{a}\right)^2\frac{C_F^2\beta_0^2\alpha_s^4}{4\pi^2}\frac{\partial^2}{\partial\nu\partial\lambda}(R_{10},\rho^\lambda P_{10}\frac{1}{E^{(0)}-H^{(0)}}P_{10}\rho^\nu R_{10})$$

Using our formulas here we find

$$-m\frac{C_F^2\beta_0^2\alpha_s^4}{4\pi^2}\frac{3+3\gamma_E^2-\pi^2+6\zeta_3}{12},$$

in agreement with the result of ref. 5, obtained with a completely diferent method (Green's functions). Secondly, we can particilarize the calculation here for $\nu=\lambda=-1$. We get

$$\delta^2_{(-1,-1)}R_{10}=\left(\tfrac{3}{4}-\tfrac{3}{4}\rho+\tfrac{1}{8}\rho^2\right)\left(\frac{ma^2}{4}\right)^2R_{10}-\tfrac{3}{8}R_{10}$$

and the last term is the normalization correction. This is in agreement with the direct result

$$\delta^2_{(-1,-1)}R_{10}=\left(\tfrac{3}{8}-\tfrac{3}{4}\rho+\tfrac{1}{8}\rho^2\right)\left(\frac{ma^2}{4}\right)^2.$$

With these evaluations we can get the result of the second order perturbation by $\rho^{-1}\log\rho$. Write

$$\delta^{(2)}_{(\rho^{-1}\log\rho)}R_{10}=\frac{\partial^2}{\partial\lambda\partial\nu}\delta^2_{(\lambda\nu)}R_{10}\equiv\left(\frac{ma^2}{4}\right)^2R_{10}\left[d_1-d_2+d_{\mathrm{norm.}}\right].$$

One defines

$$\begin{aligned}N_0\equiv&\frac{\partial^2}{\partial\lambda\partial\nu}S_{\lambda\nu}\big|_{\lambda=\nu=-1}=\frac{\pi^2}{2}+2\zeta_3-5\\
&+2\sum_{k=1}^{\infty}\left\{2\frac{\psi(k+2)-\psi(2)}{k(k+1)(k+2)}\left[\frac{1}{k}+\frac{1}{k+1}+\frac{1}{k+2}\right]+4\frac{\psi(k+2)-\psi(2)}{k^3}\right.\\
&\left.+\frac{\psi(k+3)-\psi(2)}{k(k+1)}\left[\frac{k+2}{k}+\frac{1}{k+1}\right]-2\frac{\psi'(k+2)}{k(k+1)(k+2)}-2\frac{\psi'(k+2)}{k^2}-\frac{(k+2)\psi'(k+3)}{k(k+1)}\right\}\\
&\simeq 10.29;\\
N_1\equiv&\frac{\partial^2}{\partial\lambda\partial\nu}\Psi(\lambda,\nu)\Big|_{\lambda=\nu=-1}\simeq 6.82\end{aligned}$$

(the exact value of the last given in (A5)). Moreover,

$$\frac{\partial^2}{\partial\lambda\partial\nu}\Phi(\lambda,\nu)\Big|_{\lambda=\nu=-1}=\sum_{j=1}^{\infty}\frac{\psi(j+2)-j\psi'(j+2)}{j^2}=\zeta_3+1-\frac{\pi^2\gamma_{\mathrm{E}}}{6}. \tag{A9a}$$

Some of the sums in the numbers N_i are simplified in terms of the following harmonic sums[11]:

$$\sum_{j=1}^{\infty}\frac{1}{j^2}\sum_{k=1}^{j}\frac{1}{k}=2\zeta_3;\qquad \sum_{j=1}^{\infty}\frac{1}{j^3}\sum_{k=1}^{j}\frac{1}{k}=\pi^4/18;$$

$$\sum_{j=1}^{\infty}\frac{1}{j}\sum_{k=1}^{\infty}\frac{1}{(k+j)^2}=\zeta_3;\qquad \sum_{j=1}^{\infty}\frac{1}{j^2}\sum_{k=1}^{\infty}\frac{1}{(k+j)^2}=\pi^4/120.$$

Then,

$$
\begin{aligned}
d_1 =& -\tfrac{1}{2}\left\{(1-\gamma_{\rm E})\left[\frac{2}{3}\pi^2+6\gamma_{\rm E}-\tfrac{11}{4}\right]-\tfrac{1}{2}\left(1+\frac{\pi^2}{3}\right)^2-3\left[\zeta_3+1-\frac{\pi^2\gamma_{\rm E}}{6}\right]+N_1\right\};\\
d_2 =& -\tfrac{1}{4}(1-\gamma_{\rm E})\left\{-\tfrac{19}{2}+6\gamma_{\rm E}+4\zeta_3\right\};\\
d_{\rm norm.} =& -\tfrac{3}{8}(1-\gamma_{\rm E})^2+\tfrac{5}{8}(1-\gamma_{\rm E})+\tfrac{1}{2}\left(\tfrac{1}{2}+\frac{\pi^2}{6}\right)^2-\tfrac{1}{4}N_0.
\end{aligned}
\qquad (\text{A9b})
$$

Finally, the coefficient $c_{L,1}^{(2)}$ is

$$c_{L,1}^{(2)} = d_1 - d_2 + d_{\rm norm.} \simeq 1.75. \qquad (\text{A9c})$$

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